PFAS Signature® Advanced Analytics Tool

Source Discrimination and Delineation of AFFF vs Non-AFFF Using HRMS Analysis

Per- and polyfluoroalkyl substances (PFAS) are a large class of chemicals widely used for many commercial and industrial applications, including aqueous film forming foams (AFFF), metal plating, plastic molds, photographic films, semiconductors and textile manufacturing. Many of these substances end up in the wastewater treatment plants (WWTPs) and landfills, which means these facilities also serve as potential sources of PFAS.

By understanding the specific signature of these analytes in different matrices, we can deduce information about their sources. This chemical forensic approach is not possible using the targeted analysis alone.

PFAS groundwater and soil contamination at impacted sites often cover large areas and may include co-mingled sources. There is a significant need to understand the source attribution and delineations to determine the fate and transport of these chemicals. In addition, at many of these sites, it has become a critical need for source tracking and differentiation of AFFF sources from non-AFFF sources.

OUR SOLUTION

The Battelle-developed PFAS Signature® advanced analytical tool offers PFAS source differentiation and tracking using high-resolution mass spectrometry (HRMS) techniques, in combination with PFAS targeted analysis and advanced statistical analysis.

The identification of sources of contamination is based on:

- Chemical signature
- Isomeric profiles
- Manufacturing
- Age of release
- Fate and transport
- Transformation products

SOURCE DIFFERENTIATION

Battelle has built a mass spectral PFAS source library based on PFAS targeted analysis and HRMS analysis of different PFAS sources that can be applied to a site investigation to understand the source attribution of the substances. The developed library is used to compare and differentiate the PFAS composition and trends seen in field-derived samples during a site investigation.

Our PFAS Signature tool was applied to the environmental samples collected from different source scenarios. The results show clear delineation of different sources (Figure 1).

PFAS Signature Features

- Battelle-generated database of 495 PFAS, including most of the 160 listed under EPA's Toxics Release Inventory (TRI)
- PFAS EPA ToxCast Chemical Inventory: 430 PFAS included in EPA's expanded inventory
- Battelle-generated library of different sources
- Unique data filtering to identify homologs

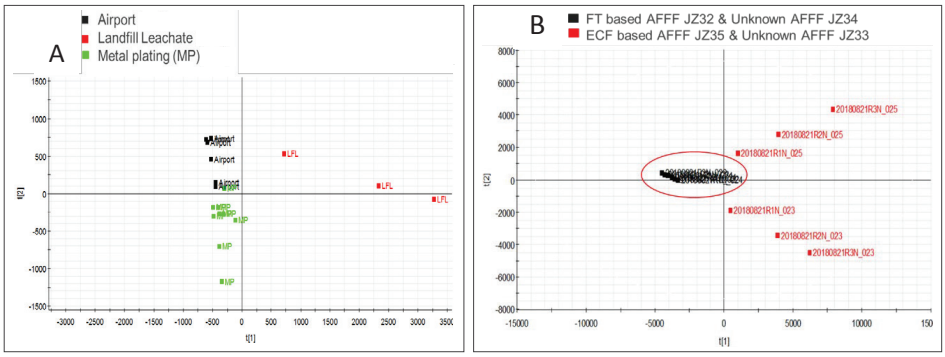

Figure 1. Example of PFAS Signature® Chemical Forensics results showing samples collected from (A) different environmental sources, and (B) AFFFs from known and unknown manufacturing sources.

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SOURCE TRACKING

Another application of our PFAS Signature tool is in a higher-level source discrimination screening. An example showing the differentiation of AFFF and non-AFFF sources is shown in Figure 2 . The cluster of non-AFFF related samples collected from different locations clearly differentiates from the AFFF-impacted environmental samples collected from different sites. The non-AFFF samples shows sources of WWTP related and the landfill leachate samples collected from different parts of United States.

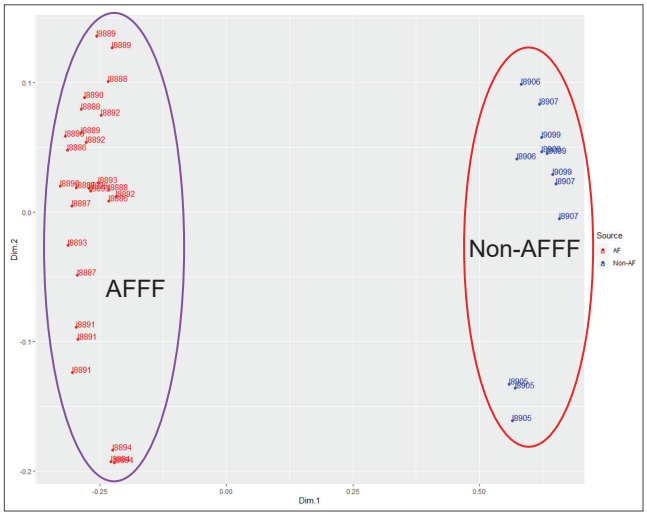

Figure 2. Multi-dimensional scaling plot showing clear differentiation of AFFF and non-AFFF sources. Plot shows HRMS PFAS data collected from different sources of non-AFFF and AFFF-impacted samples.

THE RESULTS

The information obtained from multiple lines of evidence is investigated to understand the PFAS sources and compare them.

Table 1 shows the frequency counts of the analyte specific source classification in Battelle's PFAS Source Library. Further, the following multiple lines of evidence are assessed to differentiate the sources:

- Targeted analysis
- High resolution mass spectral analysis
- Statistical analysis
- Isomer patterns
- Transformation Products

The sample E and F shows all the common PFAS analyte detections without any specific AFFF related source signature. Further, although Sample E shows 11 AFFF and 11 waste sector-related analytes, these are common transformation products between these two sources, and the lack of any other AFFF related signature, confirms the sample as non-AFFF.

Sample IDs	AFFF	Commercial Products	Waste Sector	Common Analytes
Sample A	105	11	35	50
Sample B	50	0	14	57
Sample C	18	0	5	17
Sample D	13	0	9	41
Sample E	11	0	11	50
Sample F	0	0	0	35
Sample G	55	0	13	59
Sample H	18	0	6	56
Sample I	118	14	29	76

Non-AFFF

Table 1. Frequency counts for source classifications in Battelle's PFAS source library. Source discrimination based on additional lines of evidence.

These results demonstrate that the application of Battelle's PFAS Signature approach, which is a combination of advanced HRMS tools and statistical analysis, shows great promise in understanding the source delineations and categorizations that are not possible using only targeted PFAS analysis by LC-MS/MS methods.

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